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Structures of gold Clusters: ordered, disordered isomers and transitions among them

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金クラスターの構造と構造転移

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有限個数の原子によって形成される構造は構成原子数の増加に伴って複雑に変化し、クラスター、及びクラスターの集合体の物性に影響する。我々は Gupta 多体ポテンシャルを用いた遺伝アルゴリズムにより Au_n (n=38～55) の基底状態における構造を研究した。

基底状態の構造はほとんどの場合に無秩序だが、対称性を持つ構造（秩序状態）とのエネルギー的な差は小さい。原子数の増大に伴い、秩序状態のうちで最も安定な構造は最密充填から、擬二十面体構造へと変化する。Au_{55} の動的シミュレーションの結果から、融点より低い温度において対称性の異なる構造転移（正八面体から擬二十面体、及び無秩序状態への転移）を確認した。

The study of metal clusters has flourished in the decades, motivated by the growing interest in the evolution of physical properties from the atom to the bulk solid, a progression passing through the domain of atomic clusters, as well as the seductive application potential on a broad territory like magnetic materials, catalysts, electronic nanodevices and biosensors. One of the fundamental missions for both experimental and theoretical studies on cluster is to clarify the most stable geometrical structures of nanoclusters since any macroscopic properties of cluster assembled materials maybe influenced by the atomic arrangement in cluster.

Here we present our work with semi-empirical mode on studying stable structures of gold clusters and thermal behaviors of the low temperature optimal structures of Au_{55}, which are regarded as the key elements to the alterable exotic properties of clusters and the fabrication of nano-materials.

By using the genetic algorithm, a proved powerful tool for structural optimization [1], with a Gupta many-body potential [2], we studied geometric structures of the ground states and near ground ordered states of medium-sized Au_n (n from 38 to 55) clusters. Our results confirmed the complexity of potential energy surface (PES) for metal clusters with diameter near 1 *nm*, the most stable configurations for $Au_{38\text{-}55}$ are mainly disordered with the ordered isomers very close in energy to the ground state. The lowest-lying ordered structures for clusters with atoms near 38 and 55 are close packed mode and icosahedron-like respectively, the conversion between these two distinct packing modes was found to happen with reversal while n=49, 50 and 51. A

common neighbor analysis (CNA) [3], which can quantitate the characteristic local microstructure of atom-pairs, was applied to demonstrate the disorder of the ground state configurations and the structural evolvement of the ordered isomers with increasing cluster size.

Based on the second moment approximation of tight-binding potential (TB-SMA), we performed molecular-dynamics (MD) simulations on the thermodynamical behaviors of two metastable isomers, the cuboctahedron and icosahedron, together with the less ordered ground state configuration of Au_{55} cluster. Both the metastable ordered isomers in our study undergo solid-to-solid structure transformations at low temperature, and advance to solid-liquid transition with the more stable configurations they reached. Compared with cuboctahedron, the icosahedral structure is a feasible alteration when temperature rises, however, we found further transitions into less ordered states with lower cohesive energy for icosahedron; the latter deformation, which has not been demonstrated in simulation on clusters with concerned size, is consistent with the observed disorder of small supported gold clusters (<10Å in diameter) by the reported HRTEM (high resolution transmission electron microscopy) [4] and STM (scanning tunneling microscopy) studies. Three types of solid-solid transitions are obtained: collective distortion (I), single atom migration (III), as well as local rearrangement (II). Both the partial reconstruction (II and III) and the whole shape adjustment (I) modes of small supported particles (with greater size discussed here) have been observed by means of quasimelting process in the electron-microscopic studies. Another point we found in our simulation is that the cohesive energies of the system go smoothly without any significant barrier during solid-solid transitions which implies the complexity but less abrupt of the PES. This confirms the feasibility of the suggested model [5] about vibration induced structural isomerization: when the system is (maybe partially) heated up, it can smoothly transform into a vicinity of the PES in a transient pattern by unrecoverable deviation from balance during random thermal vibration since the barriers among the local minima are often unapparent compared with the thermal energy in present simulation.

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* Some of the figures can be found in *Physics Letters A, **267**, 403(2000);* others are available by contacting: leetx@tac.tsukuba.ac.jp